Benzoic acid, 3-methoxy-
586-38-9 | DTXSID2060410

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.96e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.37e-01

Confidence level: 6.02e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
2-Methyl-p-benzoquinone	1,4-Benzoquinone	1,4-Naphthoquinone
Measured: 2.35e-11	**Measured:** 4.60e-12	**Measured:** 3.10e-12
Predicted: 2.15e-11	**Predicted:** 5.97e-12	**Predicted:** 3.16e-11